Newton's Method: details and variants

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Newton's method has been around awhile, so there are many variants / extensions etc.

Outline:
- History / example
- Convergence revisited (multiple roots)
  - Modified Newton
  - Deflation
- Practical Newton's method
- Secant Method
- Pros / Cons of Newton

Ex. Babylonian Algo

2000+ years ago, Archimedes claimed $\frac{265}{153} < \sqrt{3} < \frac{1351}{780}$. Not bad!

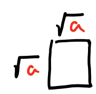
($\frac{265}{153}$: 1.73202, $\frac{1351}{780}$: 1.73205)

How did he find it? Not sure, but maybe via the Babylonian Algorithm, aka Heron's method.

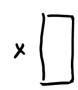
Algo: Find $x = \sqrt{a}$

Iterate $x_{n+1} = \frac{1}{2}\left(x_n + \frac{a}{x_n}\right)$

motivation:



Square w/ area a



rectangle with same area a. If one side is x, other side must be a/x.

If $x > a$ then $a/x < a$ and vice-versa

(one side too short $\Rightarrow$ other side too long)

So we have under and over approximations... so average these

It turns out this is Newton's method applied to $f(x) = x^2 - a$ (i.e. $f'(x) = 2x$)

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$$
$$= x_n - \frac{(x_n^2 - a)}{2x_n}$$
$$= x_n - \tfrac{1}{2}x_n^2 + a/2x_n = \tfrac{1}{2}(x_n + a/x_n)$$

Convergence, revisited

Recall our result from last time:

Thm: (combining Thm 2.6 and Thm 2.9)

Let $f \in C^2([a,b])$ have a root $p \in (a,b)$ with multiplicity 1 (i.e. $f'(p) \neq 0$) then if initialized sufficiently close to p, Newton's method will converge to p.

Furthermore, if additionally $|g''(x)|$ is bounded on some open interval around p, then the convergence rate is quadratic. $g(x) := x - \frac{f(x)}{f'(x)}$

Ok, but what if p isn't a simple root?

aka multiplicity 1

Def Recall, a root p of f is $\boxed{\text{multiplicity}}$ m if the 1st $m-1$ derivatives of f are 0 at p

i.e., $f(p) = f'(p) = \dots = f^{m-1}(p) = 0$ and $f^{m}(p) \neq 0$

Equivalently, if $f(x) = (x-p)^m g(x)$ and $g(p) \neq 0$

Ex: $f(x) = x(x-1)(x-2)$ has a simple root at $x=0$ (and at $x=1, x=2$) $m=1$

$f(x) = x^2(x-1)$ has a double root at $x=0$ $m=2$

$f(x) = x^3$ has a triple root at $x=0$ $m=3$

Our theorem doesn't apply. Often we still get convergence but just not at a quadratic rate

Ex $f(x) = x^2$, $x=0$ is a double root. $f'(x) = 2x$

Newton's method is $x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} = x_n - \frac{x_n^2}{2x_n} = \frac{1}{2}x_n$

i.e., $x_{n+1} = \frac{1}{2}x_n$,

so, e.g., $x_0 = 1$, then we iterate $1, 1/2, 1/4, 1/8, 1/16, \dots$

error at step n is $\frac{1}{2^n}$, $e_n = \frac{1}{2^n}$. Is this quadratic?

Check: $\lim_{n\to\infty} \frac{e_{n+1}}{e_n^2} = \lim \left(\frac{\frac{1}{2^{n+1}}}{\left(\frac{1}{2^n}\right)^2} = \frac{\frac{1}{2^{n+1}}}{\frac{1}{2^{2n}}} = \frac{2^{2n}}{2^{n+1}} = 2^{n-1} \right) = \infty$

No, not quadratic conv.

In fact, this is linear convergence since it fits the form ρ^n ($\rho = 1/2$) which we've already discussed.

One fix to this multiplicity issue is...

Modified* Newton's Method * there are many ways to modify it, this is just our book's notation

Let p be a root of f w/ multiplicity m ($m=1$ is ok, but mostly interested in $m>1$)

Define $h(x) = \frac{f(x)}{f'(x)}$. Then claim p is a root of h also

proof: $m=1$ then $f'(p) \neq 0$ so immediately $h(p) = 0$

$m>1$ then $f'(p) = 0$, $\frac{f(p)}{f'(p)} = \frac{0}{0}$ ... use L'Hôpital

so $\lim_{x\to p} \frac{f(x)}{f'(x)} = \lim_{x\to p} \frac{f'(x)}{f''(x)} = \dots = \lim_{x\to p} \frac{f^{m-1}(x)}{\underbrace{f^{m}(x)}_{\neq 0 \text{ at } p}} = 0$

Furthermore, p is a simple root of h

proof:

Can write $f(x) = (x-p)^m \cdot g(x)$ w/ $g(p) \neq 0$

then

$$h(x) = \frac{(x-p)^m g(x)}{m(x-p)^{m-1} g(x) + (x-p)^m g'(x)} = (x-p) \frac{g(x)}{m \cdot g(x) + (x-p) g'(x)} \quad \tilde{g}(p) = \frac{g(p)}{},$$

$\underbrace{\qquad\qquad}_{\tilde{g}(x)}$,

So $h(x) = (x-p)\tilde{g}(x)$ with $\tilde{g}(p) \neq 0$ $\Rightarrow$ is a simple root

$m\,g(p) + \cancel{(p-p)}g'(p)$

$= 1/m \neq 0$

... back to the point.

p is a simple root of $h(x) = \dfrac{f(x)}{f'(x)}$

So run Newton on h instead of f.

Simplifying h', we get **MODIFIED NEWTON**

$$x_{n+1} = x_n - \underbrace{\frac{f(x_n)f'(x_n)}{f'(x_n)^2 - f(x_n)f''(x_n)}}$$

ugly quotient rule stuff

Not a perfect fix:

DRAWBACKS: ① must compute f''

② subtractive cancellations

Note: wikipedia claims that if m is known, $x_{n+1} = x_n - m\dfrac{f(x_n)}{f'(x_n)}$ will work and w/ quadratic convergence

Deflation

A related idea to dealing with roots of multiplicity > 1

Suppose f has simple roots at p_1 and p_2 (if $p_1 = p_2$ it's a double root)

If $|p_1 - p_2|$ is very small, starts to act like a double root, especially w/ roundoff errors. The condition number of the root-finding problem is large

One practical consequence:

Suppose we find p_1. How to find p_2? We have to start sufficiently close to it, which is hard since we don't know where it is! We might get "sucked into" the p_1 root.

... and a fix: deflation

Define $h(x) = \dfrac{f(x)}{x - p_1}$ so h doesn't have a root at p_1, but still has a root at p_2

(this is also the name for a broader class of techniques, eg. in eigenvalue problems)

Practical Newton's method, i.e. globalization strategies

We won't go into details

① combine w/ bracketing or another root-finding method

(our book mentions a special version called False Position / Regula Falsi)

② safeguarding / linesearch:

don't let x_{n+1} go too far

(ex: if we must keep $x_n \geq 0$)

or $x_{n+1} = x_n - \alpha\dfrac{f(x_n)}{f'(x_n)}$, $\alpha \leq 1$

Need $\alpha = 1$ for quadratic convergence but often take $\alpha < 1$ for the first few iterations

Don't worry about these, just use Matlab / Scipy libraries

Secant Method

Idea: Newton's method is $x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$. What if we want to avoid calculating $f'(\,)$? *

*See future lecture on "Automatic Differentiation" ($\neq$ symbolic diff.) ex. backprop.

Well, rule-of-thumb: when a step produces an approximate result, you are free to carry it out approximately.

Since Newton's method was derived via Taylor Series, ignoring higher-order terms, lets try approximating the derivative:

$$f'(x) = \lim_{h\to 0} \frac{f(x+h)-f(x)}{(x+h)-(x)}, \text{ i.e., } f'(x_n) \approx \frac{f(x_n)-f(x_{n-1})}{x_n - x_{n-1}} \text{ if } |x_n - x_{n-1}| \text{ small}$$

(re-use our old computation)

So SECANT METHOD

$$x_{n+1} = x_n - \frac{f(x_n)\cdot(x_n - x_{n-1})}{f(x_n)-f(x_{n-1})}$$

Only needs 1 function-evaluation per step, no derivative needed. Nice!

You can extend in 2 ways:

1. use more previous points, "inverse interpolation". Not very common
2. In multi-dimensional problems, there is "more freedom", and we actually have a whole class of QUASI-NEWTON METHODS. Very useful! often "state-of-the-art"
   (names like "Broyden class", "SR1", "BFGS")
   Also, some extra computational savings that are irrelevant for scalar problems.

Convergence Analysis of Secant method

Recall for Newton $\lim \frac{|e_{n+1}|}{|e_n^2|} < \infty$ i.e. $\alpha = 2$

where $e_n = p - x_n$ is the error.

For the secant method, assuming e_n is small, we can do a Taylor expansion of our secant method iteration (tedious but straightforward) to get

$$e_{n+1} \approx \underbrace{-\tfrac{1}{2}\frac{f''(p)}{f'(p)}}_{\text{some constant}} e_n e_{n-1} \qquad (*)$$

Let's guess/hope that we have α convergence and can write

$(\forall n)$ $\underbrace{e_{n+1} = c\cdot e_n^{\alpha}}_{\text{like an "ansatz"}}$ and solve for α

then $e_{n+1} = c\cdot e_n^{\alpha} = c\cdot(c\cdot e_{n-1}^{\alpha})^{\alpha} = \text{const}\cdot e_{n-1}^{\alpha^2}$

and $e_n e_{n-1} = c\cdot e_{n-1}^{\alpha} e_n = c\cdot e_{n-1}^{\alpha+1}$

Plugging into (*) gives $e_{n-1}^{\alpha^2} = (\text{some constant})\, e_{n-1}^{\alpha+1}$ — involves c and $-\tfrac{1}{2}\frac{f''(p)}{f'(p)}$

this should be true for all e_{n-1} (when e_{n-1} is near 0)

So need (constant) $=1$

and $\boxed{\alpha^2 = \alpha + 1,}$ $\alpha > 0$ $\longrightarrow$ Solution is the Golden Ratio

$$\alpha = \frac{1+\sqrt{5}}{2} \approx 1.618$$

So... Newton's method has rate $\alpha = 2$

Secant method has rate $\alpha = 1.62$

... and in fact if you say that Newton's method takes <u>twice</u> as much work as the secant method (since you must evaluate $f(x_n)$ <u>and</u> $f'(x_n)$) then we can do <u>2</u> iterations of the secant method and count the rate as $(1.62)^2 = 2.62$

(or, keep as 1.62 but call Newton's rate $\sqrt{2} = 1.41$)

... meaning the secant method is <u>better</u> than Newton, in this sense.

Summary of Pros / Cons

Newton's method:

PROS

+ No need for bracketing interval $[a,b]$. Doesn't need $f(a)\cdot f(b) < 0$ (which excludes $f(x) = x^2$)

+ Very fast convergence eventually (the gold-standard)

+ Simple

CONS

− x_0 must be close to root, and hard to know how close. If not close enough, may diverge or converge to wrong root

− Slower convergence for multiple roots $m > 1$. Some fixes but not perfect

− practical implementations need more information, more complicated

− must supply $f'(\ )$

Secant method

Same pros / cons except no longer need to provide $f'(\ )$